

## Letters to the Editor

### Modified Bhatia's model for lattice dynamics of some b.c.c. metals

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A phenomenological model for lattice dynamics of cubic metals has been proposed by Bhatia (1955) in which the ion-ion interaction was confined to the nearest neighbours only and the electron-ion interaction was calculated using the Thomas-Fermi theory of metals. This model has been fully exploited by Joshi & Hemkar (1961, 1962) and Hemkar *et al* (1973). Recently Shukla & Camargo (1974) have pointed out correctly that Bhatia's approach to calculate the Thomas-Fermi screening parameter in terms of the elastic constants of the metal is erroneous, and gives an absurd value for this parameter. This has led Shukla & Salzberg (1973) to modify the electron ion interaction part of the dynamical matrix. While Bhatia in his model has considered the electron screening through the Thomas-Fermi theory of metals, Shukla and Salzberg's modification allowed to vary this parameter in the range predicted by the theories of Bohm-Pines and Thomas-Fermi. They have applied this theory in the case of f.c.c. metal copper and have obtained result which agrees very well with experimental findings.

The expression for the volume force obtained by Bhatia (1955) and Shukla & Camargo (1974) corresponds to the ionic centre. Physically it seems more justifiable to take an average value of the force (averaged over the whole Wigner-Seitz sphere) rather than at the ionic centre alone. With this modification we have applied this theory in the case of b.c.c. metals sodium, potassium and rubidium in the present study. The interionic interactions have been considered up to second neighbours.

The secular determinant used to determine the angular frequencies  $\omega$  of the normal modes of vibration in cubic metal can be written as

$$|D - m\omega^2 I| = 0 \quad \dots (1)$$

where  $D$  is the dynamical matrix,  $m$  is the ionic mass and  $I$  is the unit matrix

of order three. The typical diagonal and nondiagonal elements of the dynamical matrix are given by

$$D_{ii} = \frac{32}{9} (A_1 + 3B_1)(1 - C_i C_j C_k) + 4(A_2 + B_2)S_i^2 \\ + 4B_2(S_j^2 + S_k^2) + \frac{K_e q_i^2 n^{-1}}{1 + (q^2/k_c^2)} G^2(qr_0) \quad \dots (2)$$

$$D_{ij} = \frac{32}{9} A_1 S_i S_j C_k + \frac{K_e q_i q_j n^{-1}}{1 + (q^2/k_c^2)} G^2(qr_0) \quad \dots (2)$$

where  $S_i = \sin(q_i a)$ ,  $C_i = \cos(q_i a)$ ,  $a$  is the semi lattice parameter,  $q_i$  the  $i$ th component of the phonon wave vector,  $K_e$  the bulk modulus of the electron gas  $k_c = \beta(r_0/a_0)^2 K_F$ , where  $r_0$  is the radius of the atomic sphere,  $a_0$  the Bohr radius and  $K_F$  the Fermi wave vector,  $0.353 \leq \beta \leq 0.914$ .

$$G(x) = 3 \left( \frac{\sin x - x \cos x}{x^3} - \frac{1}{x} \right), \quad x = (qr_0)$$

Each set of  $A_i$ ,  $B_i$  represents force constants of the  $i$ th neighbours  $n = \frac{1}{4a^3}$  is the number of ions per unit volume

The five free parameters have been calculated by making use of the three experimental elastic constants and two zone boundary frequencies ( $\nu T_0$  and  $\nu T_2$ ) both transverse in  $[\xi, 0, 0]$  and  $[\xi, \xi, \xi]$  direction respectively). The value of  $\beta$  which gives best result is .353. The elastic constants of sodium were the same as those used by Sharma & Joshi (1963), while for potassium and rubidium these are due to measurements of Smith & Smith (1965) and Roberts & Meister (1966). The experimental frequencies for sodium, potassium and rubidium were taken from the measurements of Woods *et al* (1962), Cowley *et al* (1966) and Coplay *et al* (1973) respectively. The calculated numerical values of the force constants are given below

Constants	Sodium	Potassium	Rubidium
$A_1$ ( $10^3$ dyn cm $^{-1}$ )	3.1313	2.42705	1.91336
$B_1$ ( " )	-0.13865	-0.22217	-0.18019
$A_2$ ( " )	0.60404	1.30499	0.93694
$B_2$ ( " )	0.0355	-0.28013	-0.15413
$2aK_e$ ( " )	-0.2668	-1.62668	-1.09868

The calculated and experimental dispersion curves of sodium, potassium and rubidium are presented in figure 1. Figure 1(a) shows that there is excellent agreement between the theoretical and experimental dispersion curves for sodium

in all three directions. Figures 1(b) and 1(c) show that in the case of potassium and rubidium there is excellent agreement in all branches except one transverse branch in  $[\xi\xi0]$  direction. This deviation is attributable to the existence

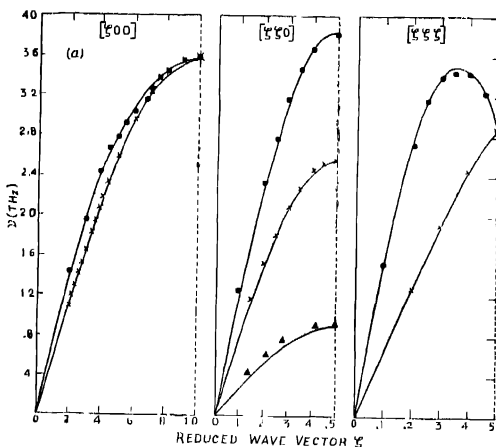


Fig. 1a

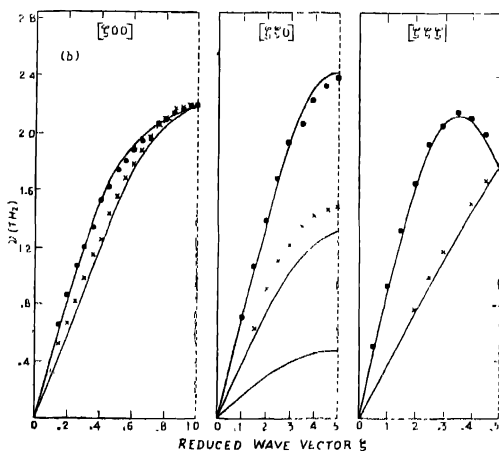


Fig. 1b

Fig. 1 Phonon dispersion curves in the three symmetry directions in sodium Fig. 1(a); in potassium Fig. 1(b) and in rubidium Fig. 1(c). The experimental points are shown by the symbol  $\bullet$  for the longitudinal branches and the symbol  $\times$  and  $\blacktriangle$  for the transverse branches

of long range interatomic forces and inherent drawback of the Bhatia's model, in which the electron gas does not modify the transverse frequencies

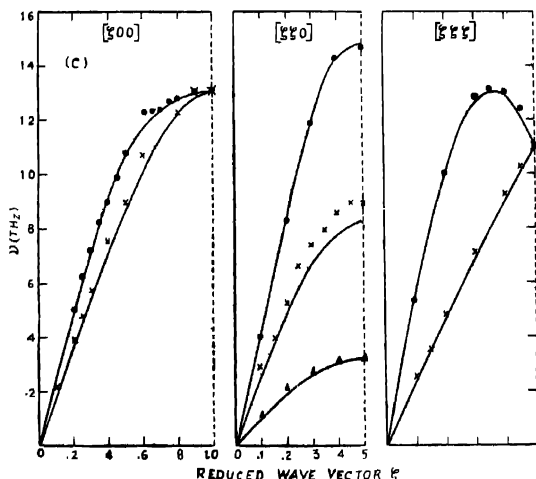


Fig. 1c

However the results presented here show that modification of Bhatia's model by extending the interionic interaction up to second neighbour with the screening parameter on the lines of Bohm and Pines and averaging the volume force over the Wigner-Seitz sphere could explain the lattice dynamics of b.c.c. metals sodium, potassium and rubidium very successfully. To further justify this approach the work on other cubic metals is in progress.

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